# DiNT: A code for direct classical energy transfer calculations, and OneDMin: A code for predicting Lennard-Jones collision parameters

## Background

Pressure dependence in chemical kinetics is almost always treated empirically and with simple models. New strategies and codes are needed to enable predictive pressure dependent kinetics.

## New theory

- Ab initio and parameterized potential energy surfaces are used in classical trajectories calculations to obtain accurate low-order moments of the average energy and angular momentum transferred due to collisions with a bath gas: $\langle \Delta E_d \rangle$, $\langle \Delta J_d \rangle$, $\langle \Delta E_d \Delta J_d \rangle$, etc…
- The moments are used to parameterize detailed models of collisions that can be used in the master equation.
- Collision rates are evaluated via effective Lennard-Jones parameters that include local anisotropy via one-dimensional minimizations.

## Codes

- `DiNT`: A general purpose trajectory code with specialized initial conditions and analysis routines for parameterizing collisional energy transfer models for use in `AITSTME`
- `OneDMin`: A stand-alone code that produces Lennard-Jones parameters for use as inputs to `DiNT` and `AITSTME`
- Availability: www.sandia.gov/~ajasper/dint
  www.sandia.gov/~ajasper/onedmin

A. W. Jasper and J. A. Miller, Combust. Flame, submitted (2013).

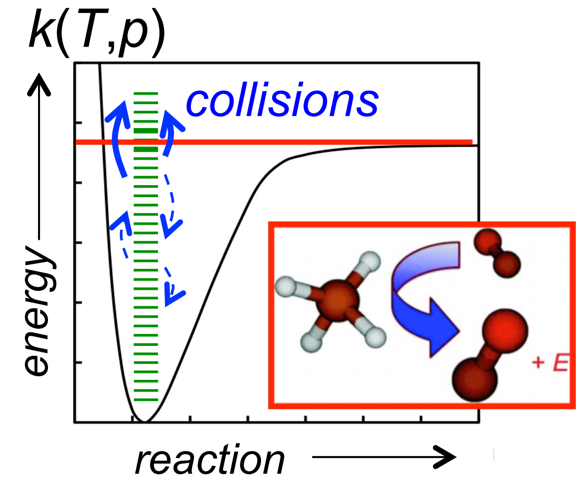


Fig 1. Bath gas collisions knock the system up and down the "energy ladder" associated with its internal states. Collisions can, e.g., energize a bound system enough to promote a unimolecular decomposition reaction. Collisions generally give rise to pressure dependence in chemical kinetics.

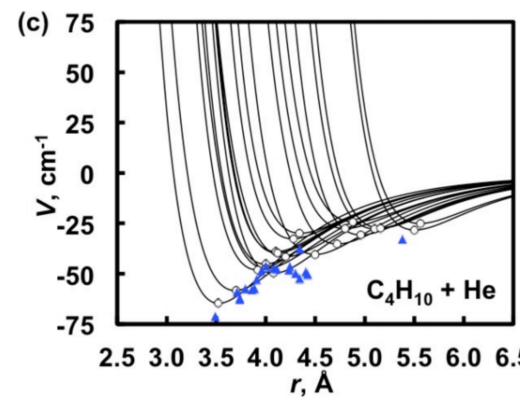


Fig. 2. The results of several one-dimensional minimizations of He approaching butane at different orientations are shown. Averaging the minima to obtain effective Lennard-Jones parameters was shown to work well for a wide variety of systems.